Three-body recombination of ultra-cold atoms to a weakly bound s level

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Abstract

We discuss three-body recombination of ultra-cold atoms to a weakly bound s level. In this case, characterized by large and positive scattering length a for pair interaction, we find a repulsive effective potential for three-body collisions, which strongly reduces the recombination probability and makes simple Jastrow-like approaches absolutely inadequate. In the zero temperature limit we obtain a universal relation, independent of the detailed shape of the interaction potential, for the (event) rate constant of three-body recombination: $\alpha_{\rm rec} = 3.9\hbar a^4/m$, where m is the atom mass.

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Three-body recombination, the process in which two atoms form a bound state and a third one carries away the binding energy, is an important issue in the physics of ultra-cold gases. This process represents the initial stage in the formation of clusters intermediate in size between individual atoms and bulk matter. Three-body recombination limits achievable densities in high-field-seeking spin-polarized atomic hydrogen [1,2] and in trapped alkali atom gases (see [3] and references therein) and, hence, places limitations on the possibilities to observe Bose-Einstein condensation in these systems.

Extensive theoretical studies of three-body recombination in ultra-cold hydrogen [1,2] and alkalis [3] showed that the rate constant of this process, $\alpha_{\rm rec}$, strongly depends on the shape of the potential of interaction between atoms and on the energies of bound states in this potential. In alkalis the recombination is caused by elastic interatomic interaction, and in the zero temperature limit $\alpha_{\rm rec}$ varies approximately as a^2 [3], where a is the scattering length for pair interaction.

All these studies, except one in spin-polarized hydrogen (see [2]), rely on Jastrow-like approximations for the initial-state wavefunction of three colliding atoms. Recent progress in the quantum three-body problem for the case where only zero orbital angular momenta of particle motion are important [4] opens a possibility for rigorous calculations of three-body recombination in ultra-cold atomic gases. In this Letter we consider the extraordinary case of recombination (induced by elastic interaction between atoms) to a weakly bound s level. The term "weakly bound" means that the size l of the diatomic molecule in this state is much larger than the characteristic radius of interaction R_e (the phase shift for s-wave scattering comes from distances $r \lesssim R_e$). In this case the scattering length is positive and related to the binding energy ε_0 by (see, e.g., [5])

$$a = \hbar/\sqrt{m\varepsilon_0} \sim l \gg R_e \tag{1}$$

(m is the atom mass), and elastic (s-wave) scattering in pair collisions is resonantly enhanced at collision energies $E \ll \varepsilon_0$. As we show, large a and l imply a rather large recombination rate constant $\alpha_{\rm rec}$. At the same time, for large positive a we find a repulsive effective

potential for three-body collisions, which strongly reduces $\alpha_{\rm rec}$. In the limit of ultra-low initial energies $E \ll \varepsilon_0$ we obtain a universal relation independent of the detailed shape of the interaction potential: $\alpha_{\rm rec} = 3.9\hbar a^4/m$.

The dependence $\alpha_{\rm rec} \propto a^4$ can be understood from qualitative arguments. For atoms of equal mass the energy conservation law for the recombination process reads

$$3\hbar^2 k_f^2/4m = \varepsilon_0, \tag{2}$$

where $k_f \sim 1/a$ is the final-state momentum of the third atom relative to the center of mass of the molecule. Recombination to a weakly bound s level occurs in a collision between two atoms, when a third atom is located inside a sphere of radius $l \sim a$ around the colliding pair. For such locations of the third atom, characterized by a statistical weight $w \sim nl^3$ (n is the gas density), this atom and one of the colliding atoms form the weakly bound state with probability of order unity. The number of recombination events per unit time and unit volume, $\nu_{\rm rec} = \alpha_{\rm rec} n^3$, can be estimated as $n^2 \sigma v (nl^3)$, where $\sigma = 8\pi a^2$ is the cross section for pair collisions. One may put velocity $v \sim \hbar k_f/m$, which gives $\alpha_{\rm rec} \sim 8\pi\hbar a^4/m$.

One can also understand qualitatively the existence of a repulsive effective potential for three-body collisions and the reduction of $\alpha_{\rm rec}$. In the mean field picture the interaction in a three-body system at (maximum of the three) interparticle separations $r \gg R_e$ can be written as $4\pi\hbar^2 n_* a/m$, where $n_* \sim 1/r^3$ is the "particle density" inside a sphere of radius r. For $a > 0$ this interaction is repulsive, which makes the statistical weight w smaller than nl^3 and decreases the numerical coefficient in the above estimate for $\alpha_{\rm rec}$. The tail of the three-body effective potential at $r \gg a$ was found in [6]. Arguments clearly showing the absence of any "kinematic" repulsion independent of the value and sign of a are given in [7].

A particular system that should exhibit three-body recombination to a weakly bound s level is a gas (or a beam) of helium atoms. The He-He potential of interaction $V(r)$ has a well with a depth of 11 K. There is only one bound state in this well, with orbital angular momentum $j = 0$ and binding energy $\varepsilon_0 \approx 1.3$ mK (see [8] and references therein). The scattering length $a \approx 100$ Å found for this potential satisfies criterion (1). The existence

of the He_2 dimer, the world's largest diatomic molecule ($l \approx 50$ Å), has been established experimentally [9]. Another system which is likely to have three-body recombination to a weakly bound s level is spin-polarized metastable triplet helium, a gas of helium atoms in the 2^3S state with spins aligned. The interaction potential [10] for a pair of spin-polarized He(2^3S) atoms supports an s level with binding energy $\varepsilon_0 \approx 2$ mK, which leads to $a \sim 100$ Å and important consequences for the decay kinetics of this system [11].

We confine ourselves to three-body recombination of identical atoms at collision energies $E \ll \varepsilon_0$ to a weakly bound molecular s level. In this case the recombination rate constant $\alpha_{\rm rec}$ can be found from the equation

$$\nu_{\rm rec} = \alpha_{\rm rec} n^3 = \frac{2\pi}{\hbar}\int \frac{d^3k_f}{(2\pi)^3}|T_{if}|^2\delta\left(\frac{3\hbar^2k_f^2}{4m} - \varepsilon_0\right)\times\frac{n^3}{6}. \tag{3}$$

Here $n^3/6$ stands for the number of triples in the gas, $T_{if} = \int \psi_i \tilde{V}\psi_f^{(0)*}d^3xd^3x'$ is the T-matrix element for three-body recombination, the coordinates $(\mathbf{x}, \mathbf{x}')$ are specified in Fig.1, ψ_i is the true wavefunction of the initial state of the triple, and $\psi_f^{(0)}$ is the wavefunction of free motion of the third atom relative to the center of mass of the molecule formed in the recombination event. Both ψ_i and $\psi_f^{(0)}$ can be written as a sum of three components, each expressed in terms of one of the three different sets of coordinates (see Fig.1):

$$\psi_i = \tilde{\psi}(\mathbf{x}, \mathbf{y}) + \tilde{\psi}(\mathbf{x}', \mathbf{y}') + \tilde{\psi}(\mathbf{x}'', \mathbf{y}''), \tag{4}$$

$$\psi_f^{(0)} = (1/\sqrt{3})[\phi(\mathbf{x}, \mathbf{y}) + \phi(\mathbf{x}', \mathbf{y}') + \phi(\mathbf{x}'', \mathbf{y}'')], \tag{5}$$
$$\phi(\mathbf{x}, \mathbf{y}) \equiv \psi_0(x)\exp(i\mathbf{k}_f\mathbf{y}),$$

where ψ_0 is the wavefunction of the weakly bound molecular state. The interaction between colliding atoms is regarded as a sum of pair interactions $V(r)$. The quantity $\tilde{V}$ is the part of the interaction which is not involved in constructing the wavefunction (5), i.e., if the molecule is formed by atoms 1 and 2 (the first term in Eq.5), then $\tilde{V} = V(\mathbf{r}_1 - \mathbf{r}_3) + V(\mathbf{r}_2 - \mathbf{r}_3)$, et cet. Using Eq.(5),

$$T_{if} = 2\sqrt{3}\int d^3xd^3x'\psi_0(x)\cos\left(\frac{\mathbf{k}_f\mathbf{x}}{2}\right)V(x')\exp(-i\mathbf{k}_f\mathbf{x}')\psi_i. \tag{6}$$

The initial wavefunction of the triple is best represented in hyperspherical coordinates. The hyperradius, defined as $\rho = (x^2/2 + 2y^2/3)^{1/2}$, is invariant with respect to the transformations $x, y \rightarrow x', y' \rightarrow x'', y''$. The hyperangles are defined as $\alpha = \arctan(\sqrt{3}x/2y)$, and similarly for α' and α''. For $E \ll \varepsilon_0$ only zero orbital angular momenta of the particle motion are important, and the wavefunction $\tilde{\psi}$ can be written as [4]

$$\tilde{\psi} = \sum_{\lambda} \frac{F_\lambda(\rho)}{\sqrt{6}} \frac{\Phi_\lambda(\alpha, \rho)}{\sin\alpha\cos\alpha}. \tag{7}$$

The functions $\Phi_\lambda(\alpha, \rho)$ are determined by the equation

$$-\frac{\partial^2 \Phi_\lambda(\alpha, \rho)}{\partial \alpha^2} + \frac{2m}{\hbar^2} V(\sqrt{2}\rho \sin\alpha)\rho^2 \left(\Phi_\lambda(\alpha, \rho) + \frac{4}{\sqrt{3}} \int_{|\pi/3-\alpha|}^{\pi/2-|\pi/6-\alpha|} d\alpha' \Phi_\lambda(\alpha', \rho)\right) = \lambda(\rho)\Phi_\lambda(\alpha, \rho), \tag{8}$$

with boundary conditions $\Phi_\lambda(0, \rho) = \Phi_\lambda(\pi/2, \rho) = 0$ and normalization $\int_0^{\pi/2} |\Phi_\lambda(\alpha, \rho)|^2 d\alpha = \pi/4$. The sum in Eq.(7) is over all eigenvalues λ corresponding to three free atoms at infinite interparticle separation. At ultra-low collision energies the lowest such $\lambda(\rho)$ alone gives a very good approximation, and we can confine ourselves to this λ. Then the function $F_\lambda(\rho)$ can be found from the (hyper)radial equation in which the quantity $\lambda(\rho)$ serves as an effective potential [4]. Under the condition $E \ll \varepsilon_0$ at interparticle distances much smaller than their De Broglie wavelength this equation reads

$$\left(-\frac{\partial^2}{\partial \rho^2} - \frac{5}{\rho}\frac{\partial}{\partial \rho} + \frac{\lambda(\rho) - 4}{\rho^2}\right) F_\lambda(\rho) = 0. \tag{9}$$

The function $F_\lambda(\rho)$ should be finite for $\rho \rightarrow 0$ and is normalized such that $F_\lambda(\rho) \rightarrow 1$ for $\rho \rightarrow \infty$.

In our case the pair interaction potential $V(r)$ supports a weakly bound s level, and the scattering length is positive and much larger than the characteristic radius of interaction R_e for this potential. For $\rho \gg R_e$ the function $\Phi_\lambda(\alpha, \rho)$ takes the form (cf. [4])

$$\Phi_\lambda(\alpha, \rho) = \begin{cases} g(\rho)\alpha\Big[\Big(\sqrt{2}\rho/a\Big)\sin(\pi\sqrt{\lambda}/2)\chi_0(\sqrt{2}\rho\alpha) + (8/\sqrt{3})\sin(\pi\sqrt{\lambda}/6)\Big], \alpha < R_e/\rho \\ g(\rho)\sin\left[\sqrt{\lambda}\,(\alpha - \pi/2)\right], \alpha > R_e/\rho, \end{cases} \tag{10}$$

where $g(\rho) = [1 + \sin(\pi\sqrt{\lambda})/\pi\sqrt{\lambda}]^{-1/2}$ and $\chi_0(r)$ is the solution of the Schrödinger equation for the relative motion of a pair of particles,

$$\left[-\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+V(r)\right]\chi_0(r)=0, \tag{11}$$

normalized such that $\chi_0 \to 1 - a/r$ as $r \to \infty$. Matching the wavefunctions (10) at $\alpha = R_e/\rho \ll 1$, to zero order in R_e/ρ we obtain the following relation for $\lambda(\rho)$ at distances $\rho \gg R_e$ (cf. [4]):

$$\frac{\sqrt{2}\rho}{a}\sin\left(\sqrt{\lambda}\frac{\pi}{2}\right)+\frac{8}{\sqrt{3}}\sin\left(\sqrt{\lambda}\frac{\pi}{6}\right)=\sqrt{\lambda}\cos\left(\sqrt{\lambda}\frac{\pi}{2}\right). \tag{12}$$

For $\rho \gg a$ this equation yields $\lambda(\rho) = 4 + 48a/\sqrt{2}\pi\rho$, and thus the potential term in Eq.(9) varies as a/ρ^3. Eq.(12) is universal in the sense that λ depends only on the ratio ρ/a, but not on the detailed shape of $V(r)$. The same statement holds for $F_\lambda(\rho)$ at distances $\rho \gg R_e$.

For infinite separation between particles, i.e., for $\rho \to \infty$ and all hyperangles larger than R_e/ρ, we have $\sqrt{\lambda} \approx 2$ and $\Phi_\lambda(\alpha, \rho) \approx \sin 2\alpha$. Accordingly, from Eq.(7) with $F_\lambda(\rho) \to 1$, each $\tilde{\psi}$ in Eq.(4) becomes equal to $\sqrt{2/3}$, and the initial wavefunction $\psi_i \to \sqrt{6}$.

The "effective potential" $\lambda(\rho)$ and the function $F_\lambda(\rho)$ for three ground-state He atoms ($a \approx 100$Å) are presented in Fig.2 and Fig. 3. The potential $V(r)$ was taken from [8]. For $\rho \gtrsim 100$Å our numerically calculated $\lambda(\rho)$ coincides (within 10%) with that following from Eq.(12), ensuring a universal dependence of F_λ on ρ/a. As $\lambda(\rho)$ is repulsive, F_λ is strongly attenuated at $\rho \lesssim a$ (see Fig.3). This leads to a strong reduction of ψ_i when all three particles are within a sphere of radius $\sim a$.

We first consider the theoretical limit of weak binding, where the scattering length a and the binding energy ε_0 are related by Eq.(1), the wavefunction of the bound molecular state at distances $x \gg R_e$ is

$$\psi_0(x) = \frac{1}{\sqrt{2\pi a}}\frac{1}{x}\exp\left(-\frac{x}{a}\right), \tag{13}$$

and the final momentum $k_f = 2/\sqrt{3}a$. From Eq.(13) one can see that the distance between the two atoms which will form the bound state should be of order a. To take away the binding energy the third atom should approach one of them to a distance of order R_e. The main contribution to the integral in Eq.(6) comes from distances $x \sim a$ and $x' \sim R_e \ll a$.

Therefore we may put $\rho \approx \sqrt{2/3}x$, $\alpha = \alpha'' \approx \pi/3$, and $\alpha' \approx \sqrt{3}x'/2x$. Then the initial wavefunction takes the form

$$\psi_i \approx (1/\sqrt{3})\chi_0(x')\tilde{F}_\lambda(\sqrt{2}x/\sqrt{3}a), \tag{14}$$

with $\tilde{F}_\lambda(z) = zF_\lambda(z)g(z)\sin(\sqrt{\lambda(z)}\pi/2)$ and $z = \rho/a$. Putting $\mathbf{k}_f\mathbf{x}'\approx 0$ and using $\int d^3x' V(x')\chi_0(x') = 4\pi\hbar^2 a/m$, from Eq.(6) we obtain $T_{if} = 48\pi^{3/2}\hbar^2 a^{5/2}G/m$, where

$$G = \int_0^\infty dz \sin(z/\sqrt{2}) \exp(-z\sqrt{3/2})\tilde{F}_\lambda(z). \tag{15}$$

The main contribution to this integral comes from $z \sim 1$ ($\rho \sim a$), where λ and F_λ (and, hence, $\tilde{F}_\lambda$) are universal functions of ρ/a. Therefore G is a universal number independent of the potential $V(r)$. Direct calculation yields $G = 0.0364$. With the above T_{if} and G, from Eq.(3) we arrive at the recombination rate constant

$$\alpha_{\rm rec} = \frac{512\pi^2 G^2}{\sqrt{3}} \frac{\hbar}{m} a^4 \approx 3.9 \frac{\hbar}{m} a^4. \tag{16}$$

The dependence $\alpha_{\rm rec} \propto a^4$, instead of $\alpha_{\rm rec} \propto a^2$, is a consequence of the recombination to a weakly bound s level and can be also obtained within the Jastrow approximation for the initial wavefunction: $\psi_{iJ} = \sqrt{6}\chi_0(\mathbf{r}_1 - \mathbf{r}_2)\chi_0(\mathbf{r}_2 - \mathbf{r}_3)\chi_0(\mathbf{r}_3 - \mathbf{r}_1)$. This approximation was proved to be a good approach for atomic hydrogen [2] and was later used for alkali atoms [3]. In our case, instead of Eq.(14), we obtain $\psi_{iJ} \approx \sqrt{6}\chi_0(x')\chi_0^2(x)$ and arrive at Eq.(16), with 4 orders of magnitude larger numerical coefficient. Such a very large discrepancy occurs because both results are determined by distances $x \sim a$, where in our (rigorous) theory ψ_i is strongly reduced by the repulsive effective potential (see above). In the Jastrow approximation this reduction is not present. Moreover, ψ_{iJ} is resonantly enhanced at distances $x < a$. Thus, for large a the Jastrow approximation gives a wrong picture of three-body collisions and is absolutely inadequate to describe recombination to a weakly bound s level.

The strong reduction of $\alpha_{\rm rec}$ due to the presence of a repulsive effective potential for three-body collisions can be treated as "quantum suppression" of three-body recombination

(see related discussions in [12,7]). Nevertheless, $\alpha_{\rm rec}$ remains finite in the zero temperature limit. In fact, due to large values of a, it is rather large. It is also worth noting that for large and *negative* scattering length the quantity $\lambda(\rho)$ should have the form of a potential well, with a repulsive core at small ρ, and the picture of recombination collisions can be completely different.

In trapped gases the kinetic energy of the third atom acquired in the recombination process usually exceeds the trap barrier, and such atoms escape from the trap. Thus, the loss rate for atoms is $\dot{n} = -Ln^3$, with $L = 3\alpha_{\rm rec}$. For three-body recombination of ground-state He atoms Eq.(16) gives $L \approx 2 \cdot 10^{-27}$ cm^6/s. As the He-He interaction has $R_e \sim 15$Å$\ll a$, this value of L is a very good approximation. More accurate calculation, using $\lambda(\rho)$ and $F_\lambda(\rho)$ determined for the He-He interaction (solid curves in Fig.2 and Fig.3), gives a correction of 10%. The same L is obtained for three-body recombination of spin-polarized He(2^3S) atoms. In this case the result is less accurate, since the characteristic radius of interaction is somewhat larger ($R_e \sim 35$Å).

Qualitatively, the picture of an effective repulsion in three-body collisions, implying a strong reduction in the recombination rate constant, can be valid for systems with positive scattering length $a \sim R_e$. One can find such systems among the ultra-cold alkali atom gases.

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FIGURES

FIG. 1. Three possible sets of coordinates for a three-body system. The relative coordinates are $\mathbf{x}$, between two particles, and $\mathbf{y}$, between their center of mass and the third particle.

FIG. 2. The "effective potential" λ as a function of ρ/a. The solid curve is obtained from Eq.(8) using the ground state He-He potential ($a = 100$Å), and the dashed from Eq.(12).

FIG. 3. The wavefunction $F_\lambda(\rho/a)$ obtained from Eq.(9). The solid curve corresponds to $\lambda(\rho)$ for the ground state He-He potential, and the dashed curve to $\lambda(\rho)$ from Eq.(12).

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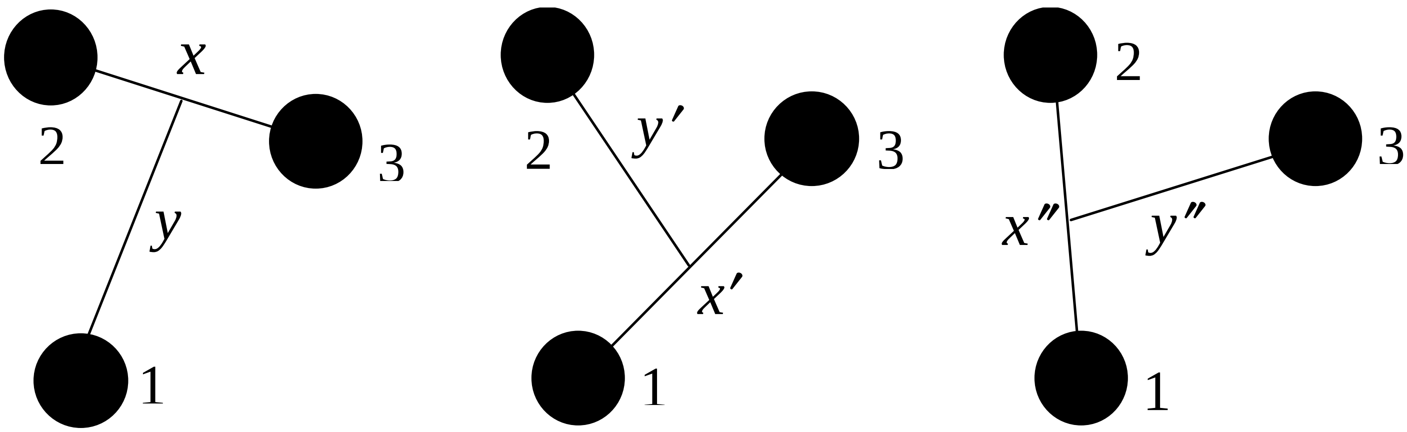
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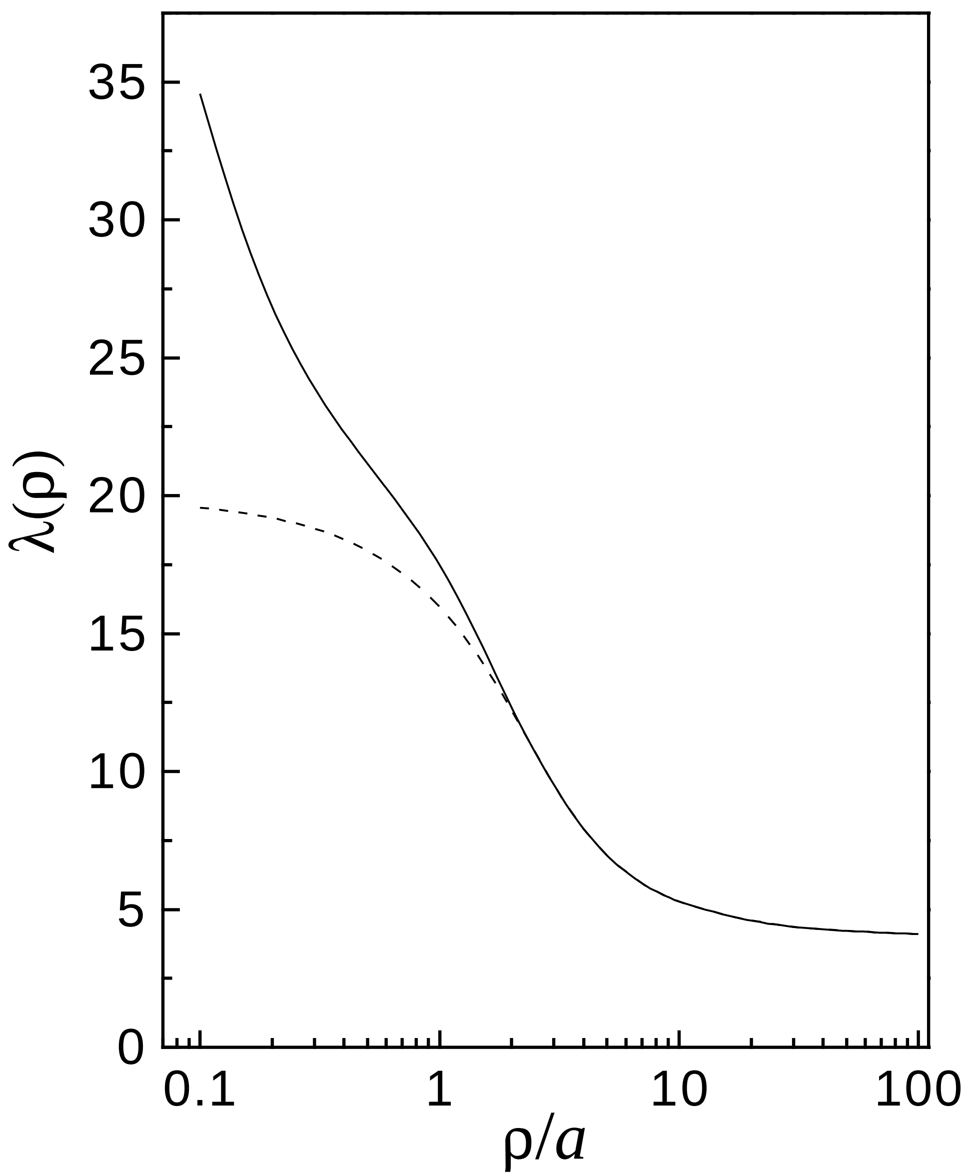

35
30
25
20
15
10
5
0
λ(ρ)
0.1
1
10
100
ρ/a